International Union of Pure and Applied Chemistry

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PROJECT SUBMISSION FORM

v. 2/2002

Any individual or group can submit a project, with or without current affiliation with an IUPAC body. Projects can be submitted at any time. For detailed information, see the additional ***Guidelines for Completion of the Project Submission Form***. Frequently Asked Questions on ***Project Submission and Approval Process*** are also available on the Union's web site at <http://www.iupac.org/projects>.

The form should be completed with a word processor and returned to the IUPAC Secretariat, preferably as an e-mail attachment at <secretariat@iupac.org>. Please do not remove section headers and answer all questions; indicate NA when a question does not apply to the proposal.

for administrative use only	*Submitted* _____ ; # _____ ***Annotated example*** *– parts of the proposal contain references to IUPAC structure and policies that are now out-of-date, but the general structure remains valid*
Date	22 Dec 1999
Project Title	Chemical Speciation of Environmentally Significant Heavy Metals and Inorganic Ligands
Series Title *(if applicable)*	
Task Group Chairman	(including address and e-mail) Professor Staffan Sjöberg Department of Inorganic Chemistry, University of Umeå, S-901 87 Umeå, Sweden e-mail: Staffan.Sjoberg@chem.umu.se **Note 1: All IUPAC correspondence is by e-mail so include an e-mail address for each member**
Task Group Members	(including address and e-mail) Professor Bob Byrne University of Southern Florida byrne@seas.marine.usf.edu Professor Kip Powell University of Canterbury, New Zealand. k.powell@chem.canterbury.ac.nz Dr. Glenn Hefter Murdoch University, Australia. Hefter@chem.murdoch.edu.au Dr. Tamas Gajda

	Attila Jozsef University, Szeged, Hungary Tamas.gajda@chem.u-szeged.hu Dr. Hans Wanner Swiss Federal Nuclear Safety Inspectorate hans.wanner@hsk.psi.ch Dr. Paul Brown ANSTO, Australia plb@ansto.gov.au **Note 2: It is necessary to indicate professional association and e-mail address for all Task Group members. It is not adequate to indicate that 'task group members will be enlisted as the project proceeds'. This would indicate that the project scope and requirements have not been adequately established.** **Note 3: Inclusion of representatives from User Groups or Industry is highly encouraged!**
Name of the person submitting this form ***if not*** *the proposed Task Group Chairman*	(including address and e-mail)
Objective	(<50 words) To provide scientists involved in chemical modelling of trace metals in environmental systems with access to the best possible (critically evaluated) equilibrium data for the reactions of these metals with major inorganic ligands.
Description	(suggest approx. 250 words) **Note 4: Put more complete details of scope of work and intended output in an appendix (one page)** The importance of considering chemical speciation (concentration of individual chemical entities) within a coherent framework is increasingly being recognised. Detailed understanding of the bioavailability and toxicity of heavy metals as well as their transport and sedimentation in natural aquifers requires knowledge of their speciation. The optimisation of many industrial processes, e.g. hydrometallurgy and pulp and paper processes, relies heavily on the understanding of chemical speciation in often-complicated multicomponent/multiphase systems. Chemical speciation modelling based on the assumption that the system is at equilibrium is frequently utilised. The validity of an assumption like this should of course always be scrutinised. However,

	it should be born in mind that the analytical techniques required for measuring trace metal (and trace metal complex) concentrations are still to a great extent missing. Thus, quite often the only option that remains is the equilibrium approach to speciation. The numerical modelling of equilibrium systems requires adequate, critically evaluated databases of numerical constants for equilibrium reactions. Access to the invaluable *IUPAC Stability Constants Database* has significantly improved the possibilities of doing literature searches for relevant thermodynamic data of metal complexes in solution. This database now contains more than 85000 records with over 18000 metal-ligand combinations. It has become obvious that the inexperienced user of a non-critical database like this runs into problems when trying to identify the most reliable data. Therefore, critical evaluation of data is necessary One responsibility of the Analytical Chemistry Division, as implied in its Terms of Reference, is to provide the scientific community with critically evaluated stability constants for metal complexes in solution. Considering the great number of metals of the Periodic Table and the increasing vast number of ligands found in our environment, this task seems insurmountable. However, the need for reliable thermodynamic data describing metal complexation as a function of temperature, pressure and ionic strength is urgent. This is true in many but not all metal – ligand systems. To satisfy the most urgent needs, priorities on selecting metal – inorganic ligand systems must be done. The present proposal puts forward a programme that identifies the most important metal ion – ligand systems from an environmental point of view. The pollutants Cu(II), Zn(II), Cd(II), Hg(II) and Pb(II), together with the inorganic ligands Cl^- , OH^-, CO_3^{2-}, $PO_4^{3-}$and SO_4^{2-}, have not yet been critically evaluated and should have highest priority. This work is seen as Part I of a series that may subsequently consider (a) data applicable to body fluids, (b) data applicable to sea water, (c) data applicable to high component concentrations and high ionic strengths as may exist in industrial processes. Besides an evaluation of soluble metal complexes in these systems, it is recommended that solubility products for pertinent solid phases be evaluated also.

Outcome (please tick box)	IUPAC Recommendation ☐ IUPAC Technical Report ☒ Other type of manuscript to be published in a journal other than *Pure and Applied Chemistry* ☐ *Specify:* …… Book ☐ Workshop or conference proceeding ☐ Set of instructional materials ☐ Database ☐ Web page ☐ Other: ……
Dissemination Plan	Provide vectors to the *PAC* article via (a) the IUPAC web site, (b) Letters to Editors of the following journals: Chemical Speciation and Bioavailability Environmental Science and Technology Aquatic Geochemistry Geochimica et Cosmochimica Acta Chemistry International **Note 5: Letter to the Editor of either Analytical Chemistry or The Analyst, or a prominent specialized Journal in the field is required.** **Note 6: The Division encourages presentation (poster or oral) at a conference of both/either interim or final product**
Relevant IUPAC Body (please tick box/boxes)	Physical and Biophysical ☐ Inorganic ☐ Organic and Biomolecular ☐ Macromolecular ☐ Analytical ☒ Environmental ☒ Human Health ☐ Nomenclature ☐ CHEMRAWN ☐ Chemistry and Industry ☐ Chemistry Education ☐ Other …… **Note 7: The Proposal is reviewed by each designated IUPAC body. The Secretariat will send Proposals to additional bodies if the content is deemed relevant to their work.**

Budget (Total from all sources)	
Travel	$4100 This will subsidise travel to two meetings, an initial planning meeting held in conjunction with the even year meeting of Commission V.6. in Lisbon (August 2000) and the second held at the IUPAC General Assembly in July 2001. It will also subsidise a meeting between the task group chairman and K. Powell to finalise the document in 2003. The proposed subsidy is: T Gajda ($700 – meetings in Lisbon and Brisbane), R Byrne ($300-Lisbon), H. Wanner ($700 – Lisbon and Brisbane), S. Sjöberg ($300- Lisbon), G. Hefter ($550-Brisbane), P. Brown ($300-Brisbane), K. Powell ($1150- Umeå). **Note 8: The apportionment of the travel budget between Task Group members, and the time and location of meetings, is required. IUPAC encourages Task Groups to meet while members are attending a Conference or similar so that travel costs can be constrained to a reasonable subsidy. Note that per diem expenses have not been requested. The budget of the Analytical Chemistry Division is limited and per diem expenses are not normally eligible for support. If the final outcome of the project is presented at a conference by the Task Group chair or a designated member of the Task Group, then arrangements should be undertaken with the conference organizers to provide an invited speaker slot, with possible financial subsidy. If a workshop or innovative conference is planned by the Task Group to bring together experts for a specific task, such as reviewing in depth the preliminary or final results of the project, then per diem expenses can be budgeted, but it is expected that the duration of such a meeting and the number of participants will be kept to a minimum.**
Administrative	Nil
Other (*describe*)	Nil
Total (in USD)	$4100
Requested from IUPAC	$4100
Requested from other Sources	Nil

External Funding Agency Applied to (if any)	-
Time Frame Planned start Date Duration of Project	 August 2000 2.5 years from initiation
Milestones	1. Prior to submission of project proposal: the proposed task group has defined the scope of work, data retrieval, responsibilities of each contributor, and criteria and correlations that will be adopted to determine reliability of data selected. **Note 9: This completed work is summarised in the Appendix and should be read as part of this proposal.** 2. August 2000: meet (in conjunction with even year meeting of Commission V.6. in Lisbon) to initiate project, to determine the structure of the manuscript and to refine criteria for data validation. 3. February 2001. Complete literature searches and selection of most authoritative publications. 4. July 2001: Complete preliminary drafts of manuscript components from each contributor. Distribute for initial review and discussion at the IUPAC General Assembly. 5. February 2002: Distribute second drafts of manuscript components. 6. Fall 2002: Compile and edit aggregated document. 7. Winter 2002: submit completed document to Analytical Chemistry Division for review. 8. Spring 2003: submit final manuscript to IUPAC for external review and publication. **Note 10: There should be clear evidence of advance planning of the project and of the process that will be used. Appendix A provides such an example.**
Anticipated Impact	Improved modelling of speciation in environmental systems. The publication will be so constructed that it not only reports the recommended values but also alerts the less experienced user to factors that must be considered when setting up speciation calculations.
Criteria for Retrospective Evaluation	Use of Science Citation Index 2-3 years after publication of the project.

Suggested Referees	(at least 3 names, including address and e-mail) **Note 11: At least three, but preferably four, external referees should be proposed. The Division President may also appoint additional or alternative referees of his choice if it is appropriate. e-mail addresses should be provided as all reviewing is done via e-mail.**

Appendix - *Chemical Speciation of environmentally significant heavy metals and inorganic ligands.*

1. The task group involved in this project are Staffan Sjöberg, Glen Hefter, Hans Wanner, Kip Powell, Paul Brown, Bob Byrne and Tamas Gajda.

2. The project will involve a detailed analysis of the most reliable papers for each metal-ligand system. In this respect it will differ from 'traditional' assessments by Commission V.6. i.e. it will not seek to establish Recommended, Provisional and Rejected values.

3. The Task Group has agreed on the scope of the work and the methods to be used in analysis, as set out below.

Scope of work

1. The project will determine a set of recommended stability constants ($\beta_{p,q}$, K_{s0}) applicable to environmental waters at low ionic strength. Recommended values for I = 0.0 M and T = 25^{o}C will be tabulated.

2. The cations will be H^{+}, Cd^{2+}, Cu^{2+}, Pb^{2+}, Zn^{2+}, Hg^{2+}, Hg_2^{2+} (CH_3Hg^{+} ?).

3. The anions will be Cl^{-}, OH^{-}, CO_3^{2-}, PO_4^{3-}, SO_4^{2-}. The Cl^{-} data may be limited to Cd, Pb and Hg, as chloride complexes with the other metal ions are rather weak.

4. This project is envisaged as Part I of a series in which other parts may consider data valid for higher ionic strengths, concentrations and temperatures: (i) data applicable to body fluids, (ii) data applicable to sea water, (iii) data applicable to high ionic strengths and high [component].

Method

1. SC-Database will be used as the initial and principal source of stability constants. Kip Powell will access and provide these data and references.

2. All members of the task group will receive a print out from SC-Database and will be asked to add important references that they are aware of.

3. Each member of the task group will accept responsibility for one part of the project. (This may involve a single ligand with all the metal ions, but the work will be divided equitably.) They will supplement the database as relevant.

4. For each metal/ligand combination we will:

(a) identify the most reliable publications/stability constants/solubility products;
(b) establish correlations between the stability constants from (a) on the basis of ionic strength dependence;
(c) identify and reject outliers;
(d) use a clearly defined ionic strength expression to establish recommended values of $\beta_{p,q}$ and K_s at I = 0 M.
(e) identify the most reliable data for ΔH for each metal-ligand combination;
(f) establish recommended values of ΔH at 25 ^{o}C and I = 0.0 M.
(g) establish the most reliable values for K_{s0}.

Outputs

1. A Table of the recommended log β, ΔH and log K_{s0} values for I = 0.0 M and T = 25^{o}C.
2. Plots of log β vs. I and log β vs. T for each (or selected) metal-ligand combinations.
3. Clear instruction on how to correct data to I $\neq$ 0 M and T $\neq$ 25 ^{o}C. At least one plot showing the effect of I on the calculated speciation and the effect of T on the speciation.

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Guidelines for Completion of Project Submission Form

Introduction

IUPAC has long been recognized as the world authority on chemical nomenclature, terminology, standardized methods for measurement, atomic weights and many other critically evaluated data. Projects sponsored by IUPAC should address one of the goals listed in the IUPAC Strategic Plan. The Strategic Plan can be downloaded from the IUPAC web site <http://www.iupac.org> or a copy can be requested from the Secretariat. After completion, the Project Submission Form should be returned to the IUPAC Secretariat, **not** to any other person or body in IUPAC. The Secretariat will initiate the review process, and communicate with the relevant IUPAC Body(ies).

While there is no set schedule for the evaluation process, it is *usually* not expected to take more than four months. Decisions will be taken during the course of the year as projects are submitted and the necessary information has been gathered. Frequently Asked Questions on ***Project Submission and Approval Process*** are also available on the Union's web site at <http://www.iupac.org/projects>

Guidelines

Project Title
Short descriptive title of project. If applicable, specify ***Series Title***

Task Group Chairman
Name and affiliation of person(s) who will be coordinator for the project.

Task Group Members
Names and affiliation of the task group members who have committed themselves and agreed to work on the project.

Objective
Describe the objective of the project in one or two sentences (<50 words). The objective should explain the value of the project to the field of chemistry involved.

Description
The description should be relatively brief (approx. 250 words) and should enable the reader to understand the purpose and methods used in the project. It has to be made clear why the project should be carried out under the auspices of IUPAC.

Include a clear statement of (a) any previous or concurrent work done on the proposed project, including conferences or workshops; (b) any previous, concurrent or planned interactions with bodies outside IUPAC that are relevant to the project.

If it is considered necessary to provide additional background information and supporting documentation to permit proper evaluation of the proposal, this should be given on a separate sheet. For help in deciding what information to include, please consult the "*Advice for Project Reviewers*" at <http://www.iupac.org/projects>.

Outcome
Is the final product of the project a recommendation or report to be published in *Pure and Applied Chemistry*, in another journal or a book, as a workshop or conference proceeding, a set of instructional materials, a web page?

What plans have been made to promote international consensus, particularly if the project results in nomenclature recommendations (including terminology, symbols, and units)?

If a book is planned, has a publisher been approached?

See also Appendix III of IUPAC Handbook *"Procedures for publications of IUPAC technical reports and recommendations*", available online as <http://www.iupac.org/reports/provisional/procedure.html>

Dissemination Plan
Identify the intended audience/stakeholders.

Explain how will the results of this project be disseminated to the affected community. How will nomenclature recommendations, for instance, be made known to practitioners or to the intended audience? A good dissemination plan is a vital part of the project.

Relevant IUPAC Body
Suggested name of the Division(s) and/or Standing Committee(s) that should review and supervise this project.

Budget
The budget should justify all planned expenditures (from all sources) over the lifetime of the project. Costs for dissemination of the results should be included. These costs might include holding a workshop (*See note at the end for definition of workshop*) or special symposium at a Conference to publicize the results of the project. Travel expenses include total costs for attending meetings of the task group, according to the rules governing IUPAC expenses (Apex airfare, IUPAC per diem according to location). Because funds are limited, every effort should be made to utilize electronic communications in lieu of meetings of the task group. In view of the modern means of electronic communication, overhead expenses are expected to be minimal. However, in some cases, costs for meeting facilities, software development, technical assistance might be accepted. Please note that IUPAC projects are not intended to be original research projects and the cost of new research work should not be a part of the project costs. In specific and well-documented cases, support for a workshop might be acceptable.

External Funding Agency Applied to (*if any****)***
When the proposer has already received funding by other organizations and is approaching IUPAC for additional funding, this should be mentioned under the previous section ***Budget.***

The proposer may also suggest in this proposal that IUPAC apply for external funding for the project, either to replace or to augment IUPAC money. This can then be considered after the review process has been completed.

Time Frame
Indicate the planned start and completion dates of the project. The expected duration of IUPAC projects is two to three years. Longer term projects should be broken into phases. Each phase should have an interim report. Projects need not conform to the IUPAC biennial budget cycle. That is, a project can begin at any time in one biennium and end in another.

Milestones
Major milestones, such as completion of first drafts of a report, dates of task group meetings should be given.

Upon acceptance of the project, the milestones will be reviewed and a specific timeline for progress reports will be agreed on with the responsible Division or Standing Committee.

Anticipated Impact
How will the results of the project affect practitioners?

Criteria for Retrospective Evaluation
How should the success of the project be measured and when? For instance, have recommendations been adopted by journals as part of their instructions for authors? Should the project impact be evaluated in one year or three after completion?

Suggested Referees
Please suggest the names (and provide address, affiliation and e-mail) of at least three external referees who can be asked to evaluate the project. Referees should be experts in the field, and in general be chosen so as to avoid the appearance of conflict of interest.

Definitions of Conference and Workshop

The following definitions are used as guides in evaluating proposals for projects.

Conference - a scientific meeting in which most participants take only a passive part in the program. Active participation is limited to the relatively few participants who present lectures or posters, chair sessions or ask questions.

Note that project funding is not intended to provide financial assistance to conferences or editing of proceedings of conferences. Under special circumstances, however, financial support for dissemination of the results of a conference may be provided. As an example, the conference may have addressed matters of global importance that result in important resolutions or other results.

Workshop - a scientific meeting in which all participants are expected to take an active part in the program. Examples include, but are not limited to:

- formulation of ideas and initial plans for projects on specific topics;
- development of recommendations or reports on specific topics;
- critical review of recommendations or reports on specific topics;
- professional development courses involving hands-on experience in new instrumental, computational or evaluation techniques.

A workshop as a part of a project can cover different aspects, such as: project initiation, recruiting of task group members, draft report and consideration of public comments, presentation and dissemination of results. It is however expected that electronic communication will be used as much as possible in various steps of development of a project.